Perlmutter performance optimization

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*This file: Perlmutter\_performance\_optimization.docx*

The purpose of this exercise is to determine the optimum run-time switches for the ASCOT5 orbit-following code on Perlmutter and to compare the performance on Perlmutter versus KNL.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| # | Group | Nmrk | .sh file | runID | --nodes | --ntasks | --cpus-per-task | OMP\_NUM\_THREADS | Wall time |
|  |  |  |  |  |  |  |  |  |  |
| 1 | group\_go\_2456 | 250,000 | perlmutter\_2456d | (none)\* | 4 | 2 | 128 | 64 | (none) |
| 2 | group\_go\_2456 | 250,000 | perlmutter\_2456e | 8825501 | 4 | 4 | 128 | 64 | 18:05 |
| 3 | group\_go\_2456 | 250,000 | perlmutter\_2456f | 8826613 | 4 | 4 | 128 | 128 | 14:34 |
| 4 | group\_go\_2456 | 250,000 | perlmutter\_2456g | 8827184 | 4 | 4 | 128 | 256 | 15:46 |
| 5 | group\_go\_2456 | 250,000 | perlmutter\_2456h | 8827230 | 4 | 4 | 128 | 512 | 16:09 |
| 6 | group\_go\_2456 | 250,000 | knl\_2456 | 3068164 | 4 |  |  | 134 | 40:33 |

Table 1. Results of run-time-switch optimization on Perlmutter for ASCOT5.

\*Note: simulation #1 was disallowed: Nodes=4 and ntasks=2 is forbidden.

All of the Perlmutter simulations use the executable:

/global/cfs/cdirs/m3195/ascot/ascot5-perlmutter-jw/ascot5/ascot5\_main\_intel

which has size = 1,787,552 and time-stamp = 9/1/2022

Comparing the fastest simulation on Perlmutter to KNL, we get a speed-up of about a factor of 2.8 which I think is about the expected speed-up (see below). I could do a similar optimization on knl, but I think the chosen value of OMP\_NUM\_THREADS (34) for the knl simulation was chosen from a previous optimization on knl. Since we are migrating to Perlmutter anyway, and since we’re getting about the right speed-up, there seems little reason to pursue this much further.

xpected performance vs knl

|  |  |  |  |
| --- | --- | --- | --- |
|  | Cori Haswell | Cori KNL | Perlmutter CPU |
| Physical cores | 32 | 64 | 128 |
| Logical CPUs per physical core | 2 | 4 | 2 |
| logical CPUs per node | 64 | 272 | 256 |
| clock speed (GHz) |  | 1.4 | 2.45 |
| NUMA domains | 2 | 1 | 8 |
| -c value for srun | floor(tpn)\*2 | floor(68/tpn)\*4 | floor(128/tpn)\*2 |

Assuming that multi-threading does not provide much performance enhancement, the ratio of performance of Perlmutter to knl would be: R = (128 \* 2.45) / (68 \* 1.4) = 3.29.